An Estimate of the Gap of the first two Eigenvalues in the Schrödinger Operator

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Dedicated to Professor Louis Nirenberg on his 75th birthday

Introduction

In my previous paper [2] with I. M. Singer, B. Wong and Stephen Yau, I gave a lower estimate of the gap of the first 2 eigenvalues of the Schrödinger operator in case the potential is convex. In this note we note that the estimate can be improved if we assume the potential is strongly convex. In particular if the Hessian of the potential is bounded from below by a positive constant, the gap has a lower bound independent of dimension. We also find gap when the potential is not necessary convex.

1 Convex potential

Let λ_1 and λ_2 be the first and second eigenvalues of the operator $\Delta - V$, and u_1 and u_2 be their corresponding eigenfunctions:

(1.1)
$$\Delta u_1 - V u_1 = -\lambda_1 u_1, \Delta u_2 - V u_2 = -\lambda_2 u_2.$$

It is well known that the first eigenfunction u_1 must be a positive function (a theorem of Courant). On the other hand, the second eigenfunction changes sign since $\int u_1 u_2 = 0$. Therefore u_2 changes sign.

One can estimate $\lambda_2 - \lambda_1$ by the following formula:

(1.2)
$$\lambda_2 - \lambda_1 = \inf_{\int f u_1 = 0} \frac{\int |\nabla f|^2 u_1^2}{\int f^2 u_1^2},$$

Here, we take another approach to derive the estimate on $\lambda_2 - \lambda_1$.

Since $u_1 > 0$, $u = \frac{u_2}{u_1}$ is a well-defined smooth function on Ω . Using the Hopf lemma and the Malgrange preparation theorem, one has the following

LEMMA 1.1. $u = \frac{u_2}{u_1}$ is smooth up to the boundary. It satisfies the Neumann condition on the boundary.

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When (1.1) are Neumann problems, Lemma 1.1 is trivial, when (1.1) are Dirichlet problems, we argue in the following way.

Note $\frac{\partial}{\partial \nu}u_1|_{\partial\Omega}\neq 0$. Therefore, by using the equation,

(1.3)
$$\Delta u = \frac{\Delta u_2}{u_1} - \frac{u_2 \Delta u_1}{u_1^2} - 2\nabla \ln u_1 \cdot \nabla \left(\frac{u_2}{u_1}\right)$$
$$= \frac{u_1 \Delta u_2 - u_2 \Delta u_1}{u_1^2} - 2\nabla \ln u_1 \cdot \nabla \left(\frac{u_2}{u_1}\right)$$
$$= -(\lambda_2 - \lambda_1) \frac{u_2}{u_1} - 2\nabla \ln u_1 \cdot \nabla \left(\frac{u_2}{u_1}\right)$$
$$= -(\lambda_2 - \lambda_1) u - 2\nabla \ln u_1 \cdot \nabla u.$$

We have the Neumann boundary condition $\frac{\partial u}{\partial \nu}|_{\partial\Omega}=0$. Let

so that

(1.5)
$$\Delta u = -(\lambda_2 - \lambda_1)u + 2\nabla \varphi_1 \cdot \nabla u.$$

THEOREM 1.1. Suppose the Ricci curvature of Ω is nonnegative and $\partial\Omega$ is convex, and

(1.6)
$$\begin{cases} \Delta u = -(\lambda_2 - \lambda_1)u + 2W \cdot \nabla u \\ \frac{\partial}{\partial \nu} u|_{\partial \Omega} = 0, \end{cases}$$

where W is a vector field such that

$$(1.7) W_{i,i} \ge \sqrt{\frac{c}{2}} > 0$$

then

(1.8)
$$\lambda_2 - \lambda_1 \ge \frac{\theta^2(\beta)}{\operatorname{diam}(\Omega)^2} + \beta \sqrt{c},$$

where $\theta(\beta) = \sin^{-1} \frac{1}{\sqrt{1 + \frac{\beta}{\sqrt{2} - \beta}}}$ and $0 < \beta < \sqrt{2}$ arbitrary.

PROOF. Consider

(1.9)
$$F = |\nabla u|^2 + \alpha u^2 \text{ with } \alpha \ge 0.$$

By computation, we have

$$(1.10) F_i = 2u_i u_{ii} + 2\alpha u u_i,$$

(1.11)
$$\Delta F = F_{ii} = 2u_{ji}u_{ji} + 2u_{j}u_{jii} + 2\alpha u_{i}u_{i} + 2\alpha uu_{ii}$$

$$= 2 |\nabla \nabla u|^{2} + 2\nabla u \cdot \nabla \Delta u + \sum_{i,j} R_{ij}u_{i}u_{j} + 2\alpha |\nabla u|^{2} + 2\alpha u\Delta u$$

$$= 2 |\nabla \nabla u|^{2} + 2\nabla u \cdot \nabla (-(\lambda_{2} - \lambda_{1})u - 2W \cdot \nabla u) + \sum_{i,j} R_{ij}u_{i}u_{j}$$

$$+ 2\alpha |\nabla u|^{2} + 2\alpha u(-(\lambda_{2} - \lambda_{1})u - 2W \cdot \nabla u)$$

$$= 2 |\nabla \nabla u|^{2} + \sum_{i,j} R_{ij}u_{i}u_{j} - 2((\lambda_{2} - \lambda_{1})|\nabla u|^{2}$$

$$+ \sum_{i,j} (W_{i,j} + W_{j,i})u_{i}u_{j} + 2\sum_{i,j} W_{i}u_{ij}u_{j})$$

$$+ 2\alpha |\nabla u|^{2} - 2\alpha((\lambda_{2} - \lambda_{1})u^{2} + 2u\nabla W \cdot \nabla u)$$

$$= 2 |\nabla \nabla u|^{2} + \sum_{i,j} R_{ij}u_{i}u_{j} - 2(\lambda_{2} - \lambda_{1} - \alpha)|\nabla u|^{2}$$

$$+ 2\sum_{i,j} (W_{i,j} + W_{j,i})u_{i}u_{j} - 2\alpha(\lambda_{2} - \lambda_{1})u^{2} + 2W \cdot \nabla F.$$

If $R_{ij} \geq 0$ and

$$(1.12) W_{i,i} \ge \sqrt{\frac{c}{2}},$$

then

(1.13)
$$\Delta F - 2W \cdot \nabla F \geq 2 |\nabla \nabla u|^2 - 2\left(\lambda_2 - \lambda_1 - \alpha - 2\sqrt{\frac{c}{2}}\right) |\nabla u|^2 - 2\alpha(\lambda_2 - \lambda_1)u^2.$$

First, we need to derive a universal lower bound for $\lambda_2 - \lambda_1$.

(1) Let $\alpha = 0$.

If F attains the maximum at the boundary point, say x_0 , then $\frac{\partial}{\partial \nu}F(x_0) \geq 0$.

Take a local orthonormal frame (e_1, \ldots, e_n) near x_0 such that $\nu = e_n$. From the definition of Hessian and second fundamental form, we have

(1.14)
$$u_{in} = e_i e_n u - (\nabla_{e_i} e_n) u$$
$$= -(\nabla_{e_i} e_n) u \text{ since } u_{\nu} = 0$$
$$= -\sum_{j=1}^{n-1} h_{ij} u_i.$$

(1.15)
$$F_{\nu} = 2\sum_{j} u_{j}u_{j\nu}$$
$$= -2\sum_{j} h_{ij}u_{i}u_{j}$$
$$\leq 0 \text{ by the convexity of } \partial\Omega.$$

This implies that $u_1 = \ldots = u_{n-1} = 0$, hence $\nabla u = 0$ at x_0 . Therefore, we have

$$F \equiv 0.$$

Thus u is a constant which is impossible.

If F attains the maximum at the interior point, say x_0 , then $\nabla u(x_0) \neq 0$. Otherwise, we have the same conclusion as above.

At x_0 ,

(1.16)
$$0 \geq \Delta F(x_0)$$

$$\geq 2 |\nabla \nabla u|^2 - 2(\lambda_2 - \lambda_1) |\nabla u|^2$$

$$+4\sqrt{\frac{c}{2}} |\nabla u|^2 \text{ since } \nabla F(x_0) = 0.$$

The last inequality is equivalent to the following:

(1.17)
$$\left((\lambda_2 - \lambda_1) - 2\sqrt{\frac{c}{2}} \right) |\nabla u|^2 \ge |\nabla \nabla u|^2 \ge 0,$$

which says that

(1.18)
$$(\lambda_2 - \lambda_1) \ge \sqrt{2c} \text{ since } \nabla u(x_0) \ne 0.$$

(2) Now, take
$$\alpha = \lambda_2 - \lambda_1 - \beta \sqrt{c} > 0$$

From the universal lower bound, we can take $\beta=\sqrt{2}-\delta$ for any small $\delta>0$ in the following argument.

Case 1. If $x_0 \in \partial \Omega$, then $\frac{\partial}{\partial \nu} F(x_0) \geq 0$.

(1.19)
$$F_{v} = 2\sum_{j} u_{j}u_{j\nu} + 2\alpha u u_{\nu}$$
$$= -2\sum_{j} h_{ij}u_{i}u_{i}$$
$$\leq 0 \text{ by the convexity of } \partial\Omega.$$

This implies that $u_1 = \ldots = u_{n-1} = 0$, hence $\nabla u = 0$ at x_0 . Therefore, we have

$$(1.20) F \le \sup \alpha u^2.$$

Case 2. $x_0 \in \overset{\circ}{\Omega}$ and

(1.21) (a)
$$\nabla u(x_0) = 0$$
.

Then by the definition

(1.22)
$$F(x_0) = |\nabla u|^2(x_0) + \alpha u^2(x_0) = \alpha u^2(x_0) < \alpha \sup u^2.$$

Hence

Case 3. $x_0 \in \overset{\circ}{\Omega}$ and

(1.24) (b)
$$\nabla u(x_0) \neq 0$$
.

Using

$$(1.25) 0 = F_i(x_0) = 2u_j u_{ji} + \alpha u u_i = 2u_j (u_{ij} + \alpha u g_{ij})$$

and rotating normal coordinates centered at x_0 , we may assume

(1.26)
$$u_1(x_0) \neq 0,$$
 $u_i(x_0) = 0, i = 2, ..., n.$

Then

$$(1.27) u_{11} + \alpha u = 0$$

which implies

$$(1.28) u_{11}^2 = \alpha^2 u^2$$

so that

Hence

$$(1.30) 0 \geq 2 |\nabla \nabla u|^2 - 2(\lambda_2 - \lambda_1 - \alpha) |\nabla u|^2 - 2\alpha(\lambda_2 - \lambda_1)u^2 + 4\sqrt{\frac{c}{2}} |\nabla u|^2$$

$$\geq -2(\lambda_2 - \lambda_1 - \alpha - \sqrt{2c}) |\nabla u|^2 - 2\alpha(\lambda_2 - \lambda_1 - \alpha)u^2$$

Then

$$(1.31) 0 \geq -2(\lambda_2 - \lambda_1 - \alpha - \sqrt{2c}) |\nabla u|^2 - 2\alpha(\lambda_2 - \lambda_1 - \alpha)u^2$$
$$= 2(-\beta\sqrt{c} + \sqrt{2c}) |\nabla u|^2 - 2\alpha\beta\sqrt{c}u^2,$$

which implies

$$(1.32) \qquad (-\beta + \sqrt{2}) |\nabla u|^2 - \alpha \beta u^2 \le 0$$

and if $\beta < \sqrt{2}$, at x_0

$$\left|\nabla u\right|^2 \le \frac{\alpha\beta}{-\beta + \sqrt{2}}u^2.$$

Hence, if $\beta < \sqrt{2}$, then at x_0

(1.34)
$$F = |\nabla u|^2 + \alpha u^2 \le \alpha \left(1 + \frac{\beta}{\sqrt{2} - \beta}\right) u^2$$

so that

(1.35)
$$F = |\nabla u|^2 + \alpha u^2 \le \alpha \left(1 + \frac{\beta}{\sqrt{2} - \beta}\right) \sup u^2,$$

which covers all the cases.

Hence

(1.36)
$$\frac{|\nabla u|}{\sqrt{\alpha(1+\frac{\beta}{\sqrt{2}-\beta})\sup u^2 - \alpha u^2}} \le 1.$$

Normalizing so that $\sup u^2 = 1$ and integrating along a shortest straight line γ from x_1 where $|u(x_1)| = \sup |u|$ to the nodal set $\{u = 0\}$, we obtain

(1.37)
$$\operatorname{diam}(M) \geq \int_{\gamma} \frac{|\nabla u|}{\sqrt{\alpha(1 + \frac{\beta}{\sqrt{2} - \beta}) - \alpha u^{2}}}$$

$$\geq \frac{1}{\sqrt{\alpha}} \int_{0}^{1} \frac{du}{\sqrt{1 + \frac{\beta}{\sqrt{2} - \beta}} - u^{2}}$$

$$= \frac{1}{\sqrt{\alpha}} \sin^{-1} \frac{1}{\sqrt{1 + \frac{\beta}{\sqrt{2} - \beta}}}$$

so that

(1.38)
$$\lambda_2 - \lambda_1 - \beta \sqrt{c} = \alpha \ge \left(\sin^{-1} \frac{1}{\sqrt{1 + \frac{\beta}{\sqrt{2} - \beta}}}\right)^2 \frac{1}{\operatorname{diam}(M)^2},$$

(1.39)
$$\lambda_2 - \lambda_1 \ge \frac{\theta^2(\beta)}{\operatorname{diam}(M)^2} + \beta \sqrt{c},$$

where

(1.40)
$$\theta(\beta) = \sin^{-1} \frac{1}{\sqrt{1 + \frac{\beta}{\sqrt{2} - \beta}}}$$

This finishes the proof of Theorem 1.1.

Formula (1.5) will satisfy the hypothesis of Theorem 1.1 if the Hessian of φ_1 has a lower bound (1.7). This will be proved in section two for convex domain.

THEOREM 1.2. For a convex domain Ω with a potential V whose Hessian has a lower bound c > 0. Then (1.8) holds.

2 Nonconvex Potential

For the first eigenfunction u_1 defined on the domain Ω in Euclidean space, we know that the Hessian of $\varphi = -\log u_1$ tends to infinity if $\partial\Omega$ is strictly convex and $u_1 = 0$ on $\partial\Omega$. Since

(2.1)
$$\Delta \varphi = |\nabla \varphi|^2 - V + \lambda_1,$$

we deduce

(2.2)
$$\Delta \frac{\partial^2 \varphi}{\partial x_i^2} = 2 \sum \left(\frac{\partial^2 \varphi}{\partial x_i \partial x_j} \right)^2 + 2 \nabla \varphi \cdot \nabla \left(\frac{\partial^2 \varphi}{\partial x_i^2} \right) - \frac{\partial^2 V}{\partial x_i^2}.$$

If $\frac{\partial^2 V}{\partial x_i^2} \ge c > 0$ in Ω , then we can argue from (2.1) that at point $x \in \Omega$ where $\frac{\partial^2 \varphi}{\partial x_i^2}$ is minimum, $\frac{\partial^2 \varphi}{\partial x_i \partial x_i} = 0$ for $j \ne i$ and

(2.3)
$$2\left(\min_{i} \frac{\partial^{2} \varphi}{\partial x_{i}^{2}}\right)^{2} \ge \frac{\partial^{2} V}{\partial x_{i}^{2}} \ge c > 0.$$

The continuity argument here was used by me in 1980 to handle the log concavity of u_1 . By looking at $tV + \frac{(1-t)c\sum x_i^2}{2n}$, we know that when t=0, $\min_i \frac{\partial^2 \varphi}{\partial x_c^2} \geq \sqrt{\frac{c}{2}} > 0$. It follows from (2.3) that this must be valid when t=1 also.

THEOREM 2.1. For a Dirichlet problem with $\frac{\partial^2 V}{\partial x_i^2} \ge c > 0$, the first eigenfunction u_1 satisfies the inequality $-\frac{\partial^2 \log u_1}{\partial x_i^2} \ge \sqrt{\frac{c}{2}} > 0$.

We shall now treat the case when V is not necessary convex. We shall assume Neumann boundary condition.

First of all, we give an upper bound for for $\Delta \varphi$. From (2.1), it is trivial to verify that

(2.4)
$$\Delta(\Delta\varphi) = 2\nabla\varphi \cdot \nabla(\Delta\varphi) + 2|\nabla\nabla\varphi|^2 - \Delta V.$$

Since $|\nabla\nabla\varphi|^2 \geq \frac{1}{n}(\Delta\varphi)^2$, we conclude that if $\Delta\varphi$ achieves its maximum in the interior of Ω ,

$$(\Delta\varphi)^2 \le \frac{n\sup\Delta V}{2}.$$

On the other hand, if $\Delta \varphi$ achieves its maximum on the boundary $\partial \Omega$,

(2.6)
$$\frac{\partial(\Delta\varphi)}{\partial\nu} \le 0.$$

From (2.1) and that $\frac{\partial \varphi}{\partial \nu} = 0$, we conclude that

(2.7)
$$\sum_{i \neq \nu} \varphi_i \varphi_{i\nu} \le \frac{\partial V}{\partial \nu}.$$

If the second fundamental of $\partial\Omega$ has eigenvalue greater than $\lambda>0$, we conclude from (2.7) that

$$\left|\nabla\varphi\right|^{2} \leq \frac{1}{\lambda} \frac{\partial V}{\partial \nu}.$$

Therefore

(2.9)
$$\nabla \varphi = |\nabla \varphi|^2 - V + \lambda_1 \\ \leq \frac{1}{\lambda} \frac{\partial V}{\partial \nu} - V + \lambda_1.$$

THEOREM 2.2. For the Neumann problem on a convex domain Ω whose boundary have principle curvature greater than $\lambda > 0$. Then either

$$\nabla \varphi \leq \frac{n}{2} \sqrt{\sup_{\Omega} \Delta V} \quad or$$
$$\Delta \varphi \leq \sup_{\partial \Omega} \left(\frac{1}{\lambda} \frac{\partial V}{\partial v} - V \right) + \lambda_1.$$

In particular for
$$\varphi = -\log u_1$$
, $|\nabla \varphi|^2 - V + \lambda_1 \leq \frac{n}{2} \sqrt{\sup_{\Omega} \nabla V}$ or $\sup \left(\frac{1}{\lambda} \frac{\partial V}{\partial v}\right) + \lambda_1$.

In order to obtain lower estimate of the Hessian of φ , we argue as follows.

For simplicity we shall assume that our domain is the ball in \mathbb{R}^n . We shall use polar coordinate so that

(2.10)
$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{n-1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta_{\theta}.$$

Therefore the operator Δ_{θ} commutes with Δ and we obtain

(2.11)
$$\Delta(\Delta_{\theta}\varphi) = 2\varphi_{r}(\Delta_{\theta}\varphi)_{r} + 2r^{-2}\sum_{i}\varphi_{\theta_{i}}(\Delta_{\theta}\varphi)_{\theta_{i}} + 2(n-2)r^{-2}\sum_{i}\varphi_{\theta_{i}}^{2} + 2\sum_{i}\varphi_{r\theta_{i}}^{2} + 2\sum_{i}\varphi_{r\theta_{i}}^{2} + 2\sum_{i}\varphi_{r\theta_{i}}^{2} + 2\sum_{i}\varphi_{r\theta_{i}}^{2} - \Delta_{\theta}V.$$

Since we assume the Neumann boundary condition, $\varphi_r=0$ along the boundary and so $(\Delta_\theta \varphi)_r=0$ along the boundary. By the sharp maximum principle, we can assume that $\Delta_\theta \varphi$ achieves its maximum in the interior of Ω which implies by (2.11) that

(2.12)
$$\sup \Delta_{\theta} \varphi \leq \frac{(n-1)^{1/2}}{\sqrt{2}} r \sup_{\Omega} (\Delta_{\theta} V)_{+}^{1/2}.$$

If we compute the upper bound of the spherical Hessian of φ , we can apply the same argument to find

(2.13)
$$\sup_{\Omega} \frac{\partial^2 \varphi}{\partial \theta_i^2} \le \frac{1}{8} + r \sup_{\Omega} \left(\frac{r \partial^2 V}{\partial \theta_i^2} \right)_+^{1/2}.$$

In order to obtain estimate of the full Hessian of φ , we use the equation

(2.14)
$$\Delta\left(\frac{r\partial\varphi}{\partial r}\right) = 2\Delta\varphi + \frac{r\partial(\Delta\varphi)}{\partial r}$$

$$= 2\Delta\varphi + 2\nabla\varphi \cdot \nabla\left(\frac{r\partial\varphi}{\partial r}\right) - 2\left|\nabla\varphi\right|^{2} - \frac{r\partial V}{\partial r}$$

$$= -2V + 2\lambda_{1} - \frac{r\partial V}{\partial r} + 2\nabla\varphi \cdot \nabla\left(\frac{r\partial\varphi}{\partial r}\right).$$

Similarly

$$(2.15) \qquad \Delta \left[r \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) \right] = 2\Delta \left(\frac{r \partial \varphi}{\partial r} \right) + r \frac{\partial}{\partial r} \Delta \left(r \frac{\partial \varphi}{\partial r} \right)$$

$$= -4V + 4\lambda_1 - 2r \frac{\partial V}{\partial r} + 4\nabla \varphi \cdot \nabla \left(\frac{r \partial \varphi}{\partial r} \right)$$

$$-2r \frac{\partial}{\partial r} (V - \lambda_1) - r \frac{\partial}{\partial r} \left(r \frac{\partial V}{\partial r} \right)$$

$$+2 \left| \nabla \left(r \frac{\partial u}{\partial r} \right) \right|^2 + 2\nabla \varphi \cdot \nabla \left(r \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) \right)$$

$$-4\nabla \varphi \cdot \nabla \left(r \frac{\partial \varphi}{\partial r} \right).$$

Hence of $r\frac{\partial}{\partial r}\Big(r\frac{\partial\varphi}{\partial r}\Big)$ achieves its maximum in the interior of Ω ,

(2.16)
$$2\left|\nabla\left(r\frac{\partial\varphi}{\partial r}\right)\right|^{2} \leq r\frac{\partial}{\partial r}\left(r\frac{\partial V}{\partial r}\right) + 4r\frac{\partial V}{\partial r} + 4V - 4\lambda_{1}.$$

Hence in this case,

$$(2.17) \sup r \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) \le \sup_{\Omega} \sqrt{\left(\frac{1}{2} r \frac{\partial}{\partial r} \left(\frac{\partial V}{\partial r} \right) + 2r \frac{\partial V}{\partial r} + 2V - \lambda_1 \right)}.$$

If $r\frac{\partial}{\partial r}\left(r\frac{\partial\varphi}{\partial r}\right)$ achieves its maximum at the boundary of Ω , we note that

$$(2.18) r \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) = \frac{\mathrm{d}^2 \varphi}{\mathrm{d}r^2} + \frac{n-1}{r} \frac{\partial \varphi}{\partial r} - \frac{n-2}{r} \frac{\partial \varphi}{\partial r}$$

$$= \Delta \varphi - \frac{1}{r^2} \Delta_\theta \varphi - \frac{n-2}{r} \frac{\partial \varphi}{\partial r}$$

$$= |\nabla \varphi|^2 - V + \lambda_1 - \frac{1}{r^2} \Delta_\theta \varphi - \frac{n-2}{r} \frac{\partial \varphi}{\partial r}.$$

Since $\frac{\partial \varphi}{\partial r} = 0$ along the boundary and $\frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) \right) \geq 0$ at the maximum point,

$$(2.19) 0 \leq -\frac{2}{r^3} |\nabla_{\theta} \varphi|^2 - \frac{\partial V}{\partial r} + \frac{2}{r^3} \Delta_{\theta} \varphi - \frac{n-2}{r} \frac{\partial^2 \varphi}{\partial r^2}$$

$$= -\frac{2}{r^3} |\nabla_{\theta} \varphi|^2 - \frac{\partial V}{\partial r} + \frac{2}{r} \left(\Delta \varphi - \frac{\partial^2 \varphi}{\partial r^2} \right) - \frac{n-2}{r} \frac{\partial^2 \varphi}{\partial r^2}$$

$$= -\frac{2}{r^3} |\nabla_{\theta} \varphi|^2 - \frac{\partial V}{\partial r} + \frac{2}{r} \left(\frac{1}{r^2} |\nabla_{\theta} \varphi|^2 - V + \lambda_1 \right) - \frac{n}{r} \frac{\partial^2 \varphi}{\partial r^2}.$$

Hence in this case

(2.20)
$$\sup r \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) \le \frac{1}{n} \sup_{\partial \Omega} \left[-r^3 \frac{\partial V}{\partial r} - 2r^2 (V - \lambda_1) \right].$$

Hence either (2.17) or (2.20) hold.

Note that since $\Delta \varphi$ is the sum of the Hessian of φ in radial and spherical directions and sum we have upper estimate of Hessian in these directions, we have also lower estimate of them in terms of $\Delta \varphi$.

THEOREM 2.3. For the Neumann problem when Ω is a ball, and $\varphi = -\log u_1$, (2.13) holds for spherical Hessian and either (2.17) or (2.20) hold for radial Hessian.

To obtain the full Hessian estimate of φ , we need to control $\varphi_{r\theta}$ and then can be accomplished as follows:

Call $\psi = r \frac{\partial \varphi}{\partial r}$. Then according to equation (2.14), we compute

(2.21)
$$\Delta(|\nabla\psi|^{2} + c\psi^{2}) = 2\sum \psi_{ij}^{2} + 2\nabla\psi\nabla(\Delta\psi) + 2c|\nabla\psi|^{2} + 2c\psi\Delta\psi$$
$$= 2\sum \psi_{ij}^{2} - 4\nabla\psi \cdot \nabla V - 2\nabla\psi \cdot \nabla\left(r\frac{\partial V}{\partial r}\right)$$
$$+4\sum \varphi_{i}\psi_{ij}\psi_{j} + 4\sum \psi_{i}\varphi_{ij}\psi_{j}$$
$$+2c|\nabla\psi|^{2} + 2c\left(-2V + 2\lambda_{1} - r\frac{\partial V}{\partial r}\right)\psi$$
$$+4c\psi\nabla\varphi\nabla\psi.$$

If $\sup(\left|\nabla\psi\right|^{2}+c\psi^{2})$ occurs in the interior, we obtain from (2.21)

$$(2.22) 0 \geq 2 \sum_{i,j} \psi_{i,j}^{2} - 4\nabla\psi \cdot \nabla V - 2\nabla\psi \cdot \nabla \left(r \frac{\partial V}{\partial r}\right)$$

$$+4 \sum_{i} \psi_{i} \varphi_{i,j} \psi_{j} + 2c |\psi|^{2}$$

$$-4cV\psi + 4c\lambda_{1}\psi - 2cr \frac{\partial V}{\partial r}\psi.$$

Note that

(2.23)
$$\sum \psi_i \varphi_{ij} \psi_j = \psi^2 \varphi_{rr} + 2\psi_r \sum \varphi_{r\theta_j} \psi_{\theta_j} + 2 \sum \psi_{\theta_i} \varphi_{\theta_i \theta_j} \psi_{\theta_j}.$$

Since we have already estimate φ_{rr} , ψ_r and $\varphi_{\theta_i\theta_j}$, we conclude that $\sum \varphi_i\varphi_{ij}\varphi_j$ can be estimated by $|\nabla\psi|^2$. By choosing C large enough, we conclude from (2.23) $|\nabla\psi|^2 + c\psi^2$ can be estimated from the information of V, ∇V and $\nabla\nabla V$.

If $|\nabla \psi|^2 + c\psi^2$ achieves its maximum on the boundary of Ω ,

$$(2.24) 0 \le 2 \sum \psi_j \psi_{j\nu} + 2\psi \psi_{\nu}.$$

Note $\psi = 0$ on $\partial \Omega$, and hence

$$(2.25) 0 \leq \sum_{j} \psi_{j} \psi_{j\nu}$$

$$= \psi_{\nu} \psi_{\nu\nu}$$

$$= \psi_{\nu} (\Delta \psi) - H \psi_{\nu}^{2}$$

$$= \psi_{nu} \left(-2V + 2\lambda_{1} - r \frac{\partial V}{\partial r} \right) + 2\varphi_{v} \psi_{\nu}^{2} - H \psi_{\nu}^{2}$$

where H is the mean curvature of $\partial\Omega$.

As $\varphi_{\nu}=0$ on $\partial\Omega$, we conclude that if $|\nabla\psi|^2+c\psi^2$ achieves its maximum on $\partial\Omega$,

$$(2.26) \psi_{\nu}^2 + c\psi^2 \le \sup_{\partial \Omega} \frac{1}{H^2} \left(-2V + 2\lambda_1 - r \frac{\partial V}{\partial r} \right)^2$$

THEOREM 2.4. If $\psi = r \frac{\partial \varphi}{\partial r}$, $|\nabla \varphi|$ can be estimated by V, ∇V , $\nabla \nabla V$ using (2.22), (2.23) and (2.25).

This completes estimates for the full Hessian of φ .

Incidently (2.14) shows that

(2.27)
$$\Delta \left(r \frac{\partial \varphi}{\partial r} - 2\varphi \right) = 2\nabla \varphi \cdot \nabla \left(r \frac{\partial \varphi}{\partial r} - 2\varphi \right) + 2\left| \nabla \varphi \right|^2 - r \frac{\partial V}{\partial r}.$$

Suppose we want to find an upper estimate of $r\frac{\partial \varphi}{\partial r} - 2\varphi$, we can proceed as follows. For any function f such that

(2.28)
$$\Delta f - \frac{1}{2} \left| \nabla f \right|^2 - r \frac{\partial V}{\partial r} \ge 0$$

we find that at an interior maximum point of $r\frac{\partial \varphi}{\partial r} - 2\varphi + f$, we have

(2.29)
$$0 \geq 2 |\nabla \varphi|^2 - 2\nabla \varphi \cdot \nabla f - r \frac{\partial V}{\partial r} + \Delta f$$
$$= 2 |\nabla \varphi - \frac{1}{2} \nabla f|^2 - \frac{1}{2} |\nabla f|^2 - r \frac{\partial V}{\partial r} + \Delta f.$$

Hence the maximum of $r\frac{\partial \varphi}{\partial r}-2\varphi+f$ must occur on the boundary of $\partial\Omega$ which is at most $\max_{\partial\Omega}(-2\varphi+f)$.

THEOREM 2.5. For the Neumann problem with $\varphi = -\log u_1$,

(2.30)
$$r\frac{\partial \varphi}{\partial r} - 2\varphi + f \le \max_{\partial \Omega} (f - 2\varphi)$$

where f is any function satisfies (2.29).

If we normalize u_1 so that $u_1 \leq 1$ on $\partial\Omega$ then $\max_{\partial\Omega}(-2\varphi) \leq 0$ and (2.30) gives a good growth estimate of φ .

For example, if $\frac{\partial V}{\partial r} \ge 0$, we can then take f=0 and (2.30) says that $\frac{\varphi}{r^2}$ is monotonic decreasing which means that u_1 decays like a Gaussian.

3 Estimate of gap for more general potential

We shall improve the estimate that we obtained in section one.

Let c be any constant greater than $\sup u$ when $u = \frac{u_2}{u_1}$. Let α be a positive constant to be determined. Then consider the function

(3.1)
$$F = \frac{|\nabla u|^2}{(c-u)^2} + \alpha \log(c-u).$$

Then

(3.2)
$$F_i = 2(\sum u_j u_{ji})(c-u)^{-2} + 2|\nabla u|^2 u_i(c-u)^{-3} - \alpha u_i(c-u)^{-1},$$

(3.3)
$$\Delta F = 2(\sum u_{ji}^{2})(c-u)^{-2} + 2(\sum u_{j}(\Delta u)_{j})(c-u)^{-1} + 8(\sum u_{j}u_{ji}u_{i})(c-u)^{-3} + 2|\nabla u|^{2}\Delta u(c-u)^{-3} + 6|\nabla u|^{4}(c-u)^{-4} - \alpha(\Delta u)(c-u)^{-1} - \alpha|\nabla u|^{2}(c-u)^{-2}.$$

Since u satisfies the Neumann condition and $\partial\Omega$ is assumed to be convex, F can not achieve its maximum at the boundary of Ω as its normal derivative would have to be positive. So we assume F achieves its maximum in the interior of Ω where $\nabla F=0$.

If $\nabla u \neq 0$ at this point, we can choose coordinate so that $u_1 \neq 0$ and $u_i = 0$ for i > 1. Then

(3.4)
$$u_{11}(c-u)^{-1} + |\nabla u|^2 (c-u)^{-2} = \frac{\alpha}{2}.$$

Hence

(3.5)
$$\Delta F \geq 2|\nabla u|^{4}(c-u)^{-4} - 2\alpha|\nabla u|^{2}(c-u)^{-2} + \frac{\alpha^{2}}{2} - 2(\lambda_{2} - \lambda_{1})|\nabla u|^{2}(c-u)^{-2} + 4(\inf \varphi_{ii})|\nabla u|^{2}(c-u)^{-2} + 4\alpha|\nabla u|^{2}(c-u)^{-2} - 2|\nabla u|^{4}(c-u)^{-4} - 2(\lambda_{2} - \lambda_{1})u(c-u)^{-1}|\nabla u|^{2}(c-u)^{-2} + \alpha(\lambda_{2} - \lambda_{1})u(c-u)^{-1} - \alpha|\nabla u|^{2}(c-u)^{-2}.$$

If we choose α so that

(3.6)
$$\alpha \ge 2(\lambda_2 - \lambda_1) - 4\inf \varphi_{ii} + 2(\lambda_2 - \lambda_1)(\sup u)(c - \sup u)^{-1},$$

(3.7)
$$\alpha > 2(\lambda_2 - \lambda_1)(\sup u)(c - \sup u)^{-1}.$$

Then $\Delta F > 0$ which is not possible. Hence at $\nabla F = 0$, $\nabla u = 0$ and we obtain

$$(3.8) \sup F \le \alpha \log c.$$

If we choose $c = (1 + \varepsilon) \sup u$ with $\varepsilon > 0$, we can choose

(3.9)
$$\alpha = 2(\lambda_2 - \lambda_1)(1 + \varepsilon^{-1}) - 4\inf \varphi_{ii}.$$

(Here we assume $\inf \varphi_{ii} \leq 0$, otherwise we can apply section 1.)

THEOREM 3.1. Choose α to be (3.9), then

(3.10)
$$\frac{|\nabla u|}{c-u} \le \sqrt{\alpha} (\log(c) - \log(c-u))^{\frac{1}{2}}.$$

Therefore

$$\left|\nabla\left(\log\left(\frac{c}{c-u}\right)\right)^{\frac{1}{2}}\right| \le \frac{1}{2}\sqrt{\alpha}.$$

Integrating this inequality from $u = \sup u$ to u = 0, we find

(3.12)
$$\sqrt{\log\left(1+\frac{1}{\varepsilon}\right)} \le \frac{1}{2}\sqrt{\alpha}d(\Omega).$$

Hence

$$\alpha \ge 4\log\left(1 + \frac{1}{\varepsilon}\right)d(\Omega)^{-2}.$$

In particular

(3.13)
$$(\lambda_2 - \lambda_1)(1 + \varepsilon^{-1}) \ge 2\log\left(1 + \frac{1}{\varepsilon}\right)d(\Omega)^{-2} + 2\inf\varphi_{ii}.$$

Hence

(3.14)
$$\lambda_2 - \lambda_1 \ge 2d(\Omega)^{-2} \exp[(\inf \varphi_{ii}) d(\Omega)^2].$$

THEOREM 3.2. Let Ω be a convex domain so that for the first eigenfunction u_1 of the operator $-\Delta + V$, the Hessian of $-\log u_1$ is greater than -a. Then the gap of the first eigenfunction of the operator $-\Delta + V$ is greater than

$$(3.15) \lambda_2 - \lambda_1 \ge 2d(\Omega)^{-2} \exp(-ad^2(\Omega)).$$

Note that we have estimate a in section 2 already and (3.15) does give a gap estimate for arbitrary smooth potential.

Note that Theorem 3.2 shows that it is possible to estimate $\lambda_2 - \lambda_1$ from below depending only on the lower bound of the Hessian of potential as long as Ω is convex and $d(\Omega)$ is finite. The estimate may not be optimal and it is possible that $d(\Omega)$ should be replaced by integral of some function.

4 Behavior of the ground state

It is clear from the above discussions that the behavior of the Hessian of the function $\varphi = -\log u_1$ is important. Since

(4.1)
$$\Delta \varphi = |\nabla \varphi|^2 - V + \lambda_1.$$

It is clear that upper estimate of $\Delta \varphi$ can be used to control the growth of φ and hence the growth of u_1 .

Clearly,

(4.2)
$$\Delta(\Delta\varphi) = 2\sum \varphi_{ij}^2 - 2\sum \varphi_j(\Delta\varphi)_j - \Delta V.$$

Let ρ be a nonnegative function which varnishes on $\partial\Omega$, then

(4.3)
$$\Delta(\rho^{2}\Delta\varphi) = 2(\rho\Delta + |\nabla\rho|^{2})\Delta\varphi + 2\rho\nabla\rho \cdot \nabla(\Delta\varphi) + \rho^{2}(2\sum\varphi_{ij}^{2} - 2\sum\varphi_{j}(\Delta\varphi)_{j} - \Delta V).$$

At the point where $\rho^2 \Delta \varphi$ achieves its maximum, $\nabla(\rho^2 \Delta \varphi) = 0$ and

(4.4)
$$\rho \nabla (\Delta \varphi) + 2(\Delta \varphi) \nabla \rho = 0.$$

Hence

(4.5)
$$\Delta(\rho^{2}\Delta\varphi) = 2(\rho\Delta\rho - 3|\nabla\rho|^{2})\Delta\varphi + 2\rho^{2}\sum_{i}\varphi_{ij}^{2} - 4\rho\Delta\varphi(\rho\cdot\nabla\varphi) - \rho\Delta V.$$

Note

$$(4.6) |\nabla \rho \cdot \nabla \varphi| \le |\nabla \rho| (\sqrt{|\nabla \varphi|^2 - V + \lambda_1} + \sqrt{(V - \lambda_1)_+}),$$

where $(V - \lambda_1)_+$ is the positive part of $V - \lambda_1$. Therefore when $\rho^2 \Delta \varphi$ achieves its maximum,

$$(4.7) 0 \geq 2(\rho\Delta\rho - 3|\nabla\rho|^2)\rho^2\Delta\varphi + \frac{2}{n}(\rho^2\Delta\varphi)^2 -4(\rho^2\Delta\varphi)|\nabla\rho|(\sqrt{\rho^2\Delta\varphi} + \sqrt{(V - \lambda_1)})_+ - \rho^4\Delta V.$$

THEOREM 4.1. For any function ρ vanishing at the boundary of Ω , $\rho^2 \Delta \varphi$ is bounded from above by $\sup(\rho \Delta \rho - 3|\nabla \rho|^2)$, $\sup|\nabla \rho|^2$, $\sup\rho^2 \sqrt{(\Delta V)_+}$ and $\sup|\nabla \rho|\sqrt{(V - \lambda_1)_+}$.

Note that if V grows at most quadratically, Theorem 4.1 shows that $\Delta \varphi$ can be bounded from above in terms of $(\Delta V)_+$. Since $\Delta \varphi = |\nabla \varphi|^2 - V - \lambda_1$, $|\varphi|$ can not grow faster than the integral of $\sqrt{(V-\lambda_1)_+}$ along paths tend to infinity. In particular for the first eigenfunction $u_1 = \exp(-\varphi_1)$, it cannot decay too fast.

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